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The Effect of Solvation on the Excited States of Water and Methanol.

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The study of the electronic structures/spectra of solvated systems is more difficult than their gas counterparts due to the complex nature of solute-solvent interactions. In this work the effects of solvation on the excited states of water and methanol are investigated. The excitation energies of the five singlet excited states of water complexed with a water molecule, and of the first three singlet excited states of methanol also complexed with one molecule of water are computed using ab initio methods: MCSCF, CASPT2, MRCI and the Coupled Cluster- Linear Response Theory, also known as Equation of Motion, EOM-CCSD. The possible solvatochromic shifts are investigated.